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On Thermalization in Classical Scalar Field Theory

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Abstract

Thermalization of classical fields is investigated in a ϕ^4 scalar field theory in $1+1$ dimensions, discretized on a lattice. We numerically integrate the classical equations of motion using initial conditions sampled from various nonequilibrium probability distributions. Time-dependent expectation values of observables constructed from the canonical momentum are compared with thermal ones. It is found that a closed system, evolving from one initial condition, thermalizes to high precision in the thermodynamic limit, in a time-averaged sense. For ensembles consisting of many members with the same energy, we find that expectation values become stationary - and equal to the thermal values - in the limit of infinitely many members. Initial ensembles with a nonzero (noncanonical) spread in the energy density or other conserved quantities evolve to noncanonical stationary ensembles. In the case of a narrow spread, asymptotic values of primary observables are only mildly affected. In contrast, fluctuations and connected correlation functions will differ substantially from the canonical values. This raises doubts on the use of a straightforward expansion in terms of 1PI-vertex functions to study thermalization.

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1 Introduction

Time evolution of correlation functions in classical field theory out of thermal equilibrium is of interest for various reasons. On one side a classical field theory (after discretization on a lattice to regulate the Rayleigh-Jeans divergence) provides a relatively simple playground for testing various ideas of statistical mechanics. Examples in the literature include the approach to thermal equilibrium [1], the relation with chaos [2], and the dynamics in thermal gradients, when the system is coupled to external heat baths at the boundaries [3]. A more pragmatic reason is given by the recent emergence of classical [4, 5, 6] and semiclassical [7] approximations to nonperturbative dynamics of low-momentum modes in nonequilibrium *quantum* field theory. Knowledge of thermalization properties of classical field theories is important to determine the applicability of these approaches.

A nonequilibrium ensemble can be defined by an initial probability distribution with the property that the energy is distributed over the available degrees of freedom in some nonequilibrium fashion. One would say that an ensemble with a very large number of degrees of freedom has "thermalized" when after sufficiently long time the expectation values of observables approach the thermal ones, and in fact become time-independent. More precisely, we restrict this criterion to observables and correlation functions with support in a region of space that is sufficiently small as compared to the total volume. (We will always consider isolated systems, i.e. without an external heat bath.) We concentrate on equal-time correlation functions, and define thermal values of correlation functions by expectation values in the canonical ensemble with the same average energy as the ensemble under consideration.

It has been argued [8, 9, 10] that the existence of conserved correlation functions constitutes an obstruction to thermalization. This may be illustrated by an ensemble consisting of many independent experiments with isolated systems where the initial conditions have some experimental uncertainty in the energy density ϵ. As an example, this is realized in heavy-ion collisions by many independent scattering events. An initial nonvanishing spread $\Delta\epsilon/\epsilon$ is conserved by the time evolution of the ensemble - it corresponds to a conserved correlation function. In consequence, the ensemble cannot relax asymptotically to a canonical ensemble with a temperature given by the average energy density. In the latter case $\Delta\epsilon/\epsilon$ would have to vanish in the thermodynamic limit. In this paper we clarify how this issue can be related to our understanding of thermalization.

For our investigation a natural ordering is provided by the type of ensembles that can be considered. Given an initial nonequilibrium probability distribution, we call one particular realization of this distribution a "microstate". The simplest ensemble consists of only one microstate. We will see below that for single microstates fluctuations in time remain, even for asymptotically large times, and

we study therefore the behaviour of time-averaged observables

$$\langle O\rangle_{\Delta t}(t) = \frac{1}{\Delta t}\int_{t-\Delta t}^{t} dt'\, O(t'). \tag{1}$$

They become stationary for sufficiently large t and Δt. We shall call this behaviour "quasi-stationary". More advanced ensembles are formed by superimposing more than one microstate: in particular, an ensemble consisting of N_m microstates which have the same energy E and contribute with the same weight will be referred to as a fixed-energy ensemble. Of interest is now the behaviour of ensemble-averaged observables,

$$\langle O\rangle_{E,N_m}(t) = \frac{1}{N_m}\sum_{i=1}^{N_m} O_i(t). \tag{2}$$

Note that these expectation values can be defined locally in time, which makes it more suitable for the study of the time evolution of expectation values out of equilibrium. Expectation values in a fixed-energy ensemble with an infinite number of microstates are denoted as $\langle O\rangle_E \equiv \langle O\rangle_{E,\infty}$. Finally, a more general ensemble can be built as the superposition of states with different energy, weighted with a weight function $f(E)$.

Specific questions can now be raised. Will the nonequilibrium ensembles described above indeed thermalize according to the definition given earlier? Are there restrictions on those ensembles, e.g. on the weight function $f(E)$? Is it important that a fixed-energy ensemble, unlike the canonical one, has no energy fluctuations? Further: is it possible to approximate the time evolution using a (truncated) expansion in, for instance, 1-particle irreducible vertex functions, at arbitrarily long times?

2 Classical scalar field theory

We will address the issues mentioned above from first principles by numerical simulations using a simple classical scalar field theory in $1+1$ dimensions with the action

$$S = \int dt \int_0^L dx \left[\frac{1}{2}(\partial_t\phi)^2 - \frac{1}{2}(\partial_x\phi)^2 - \frac{1}{2}m^2\phi^2 - \frac{\lambda}{8}\phi^4\right]. \tag{3}$$

Here L is the (one-dimensional) volume and we use periodic boundary conditions. The equation of motion reads $\partial_t^2\phi = \partial_x^2\phi - m^2\phi - \lambda\phi^3/2$, and the conserved energy is

$$E = \int_0^L dx \left[\frac{1}{2}\pi^2 + \frac{1}{2}(\partial_x\phi)^2 + \frac{1}{2}m^2\phi^2 + \frac{\lambda}{8}\phi^4\right], \tag{4}$$

where $\pi(x,t) = \partial_t\phi(x,t)$ is the canonical momentum. In order to solve the time evolution, we discretize the action in the standard way on a lattice with N spatial

lattice points, with spatial lattice spacing a (such that $aN = L$) and time step a_0, and derive the equation of motion from the discretized action.[1] We then solve this equation numerically, starting from a nonequilibrium initial condition.

Out of the infinite number of possible nonequilibrium initial conditions, we chose the following microstates: the field $\phi(x, 0)$ is initially set to zero, and only a few long wavelenghts of $\pi(x, 0)$ are excited. Explicitly,

$$\phi(x,0) = 0, \quad \pi(x,0) = \sum_k{}' A\cos(2\pi kx/L - \psi_k), \tag{5}$$

where k is integer and $0 \leq \psi_k < 2\pi$ [1]. The prime indicates that only a very restricted number $n_\mathrm{e} \ll N$ of modes is excited. We have chosen $n_\mathrm{e} = 4$ modes with momentum of the order of the mass ($p \equiv 2\pi k/L \approx m$). For arbitrary coupling constant the initial energy is $E = n_\mathrm{e} LA^2/4$. Many initial conditions with a certain energy can be generated by choosing different phases ψ_k in Eq. (5). We construct a fixed-energy nonequilibrium ensemble as a superposition of N_m microstates with random ψ_k and equal weight. The time evolution of ensemble averages can be calculated by summing over the realizations. Note that for $N_m \to \infty$, the fixed-energy ensemble defined in this way is translationally invariant: for instance the initial two-point function reads

$$\langle \pi(x,0)\pi(y,0)\rangle_E = \sum_k{}' \frac{1}{2} A^2 \cos[2\pi k(x-y)/L]. \tag{6}$$

Microstates and ensembles with $N_m < \infty$ do not have this property, of course.

The class of initial conditions (5) is far from classical thermal equilibrium, where all modes of both ϕ and π have nonzero expectation values of their squared amplitude, determined by the parameters in the action and the temperature T. For a free system ($\lambda = 0$), the temperature is related to the total energy by equipartition as $E = NT = LT/a$. Note that this reflects the (linear) Rayleigh-Jeans divergence in classical thermal field theory, as a goes to zero. Corrections due to the nonzero coupling constant are finite in $1 + 1$ dimensions.

It is convenient to use the mass parameter m as the dimensionful scale, and rescale all dimensionful parameters with m, i.e. $x = x'/m,\ t = t'/m,\ \lambda = m^2\lambda'$. If we also rescale the field with the dimensionless combination $v \equiv m/\sqrt{3\lambda}$, $\phi = v\phi'$, the classical equation of motion is independent of λ'. The dimensionless energy E' is related to unscaled energy E as $E' = E/(mv^2) = 3\lambda E/m^3$, and similar for the temperature: $E'/T' = E/T$. A given value of E' describes therefore several values of λ/m^2 if E/m is changed accordingly. Note that for fixed E/m a more strongly coupled theory is obtained by taking higher E'. To anticipate the Rayleigh-Jeans divergence in thermal equilibrium, we keep the ratio E'/N fixed, when varying the lattice spacing or volume. Besides E'/N, the remaining parameters that need to be specified are the physical volume $L' = mL$, the lattice spacing $a' = ma$ (or

[1] This gives the Lagrange version of the leap frog discretization.

equivalently $N = mL/ma$). For the time step we use $a_0/a = 0.05$ (we have also used smaller time steps, and found no significant deviations).

We concentrate on correlation functions that are built from the conjugate momentum $\pi(x,t)$, since these can easily be compared with equal-time expectation values in thermal equilibrium, where the only nontrivial correlation function is

$$\langle \pi(x,t)\pi(y,t)\rangle_T = \frac{T}{a}\delta_{xy}. \tag{7}$$

With respect to the space dependence, we consider both expectation values of global observables, i.e. observables averaged over the complete volume, and observables that are averaged in space over a "subvolume" with size $L_s < L$ only. In the latter case one may think of the rest of the system as an effective heat bath, though it is of course still correlated with the subsystem under consideration and hence not a heat bath in the strict sense.

We focus on expectation values, made from the following two building blocks:

$$G_s^{(2)}(x_s,t) = \frac{1}{N_s}\sum_x^{(N_s)}\pi^2(x,t), \quad G_s^{(4)}(x_s,t) = \frac{1}{N_s}\sum_x^{(N_s)}\pi^4(x,t). \tag{8}$$

The label N_s denotes that the average is taken over a subvolume with $N_s = L_s/a$ points, centered around $x = x_s$. In case that $N_s = N$ the complete volume average is taken, and the subscript s is omitted. The kinetic energy in a subvolume is given by

$$K_s(x_s,t) = \frac{1}{2}aN_sG_s^{(2)}(x_s,t). \tag{9}$$

In thermal equilibrium its value is $\langle K_s\rangle_T = N_sT/2$, independent of x_s of course. One may define an effective temperature, locally in time and out of equilibrium, from the expectation value

$$T_\pi(t) = 2\langle K\rangle(t)/N. \tag{10}$$

Note that this is an example of a "primary" quantity, i.e. it is directly given as an ensemble average.

The observables we investigate are the following. In the canonical ensemble π is a gaussian (free) field, which implies that $\langle G_s^{(4)}\rangle_T = 3\langle G_s^{(2)}\rangle_T^2$. We want to see whether π becomes eventually gaussian in the nonequilibrium ensembles as well. We define the deviation from π being gaussian in a subvolume as

$$\mathrm{dev}(\pi_s) = \frac{\langle G_s^{(4)}(x_s,t)\rangle}{3\langle G_s^{(2)}(x_s,t)\rangle^2} - 1. \tag{11}$$

For one microstate or in a fixed-energy ensemble the conserved total energy has no fluctuations. The time evolution of the fluctuations in the kinetic energy of subsystems

$$\mathrm{fluc}(K_s) = \frac{\langle (K_s - \langle K_s\rangle)^2\rangle}{\langle K_s\rangle^2}. \tag{12}$$

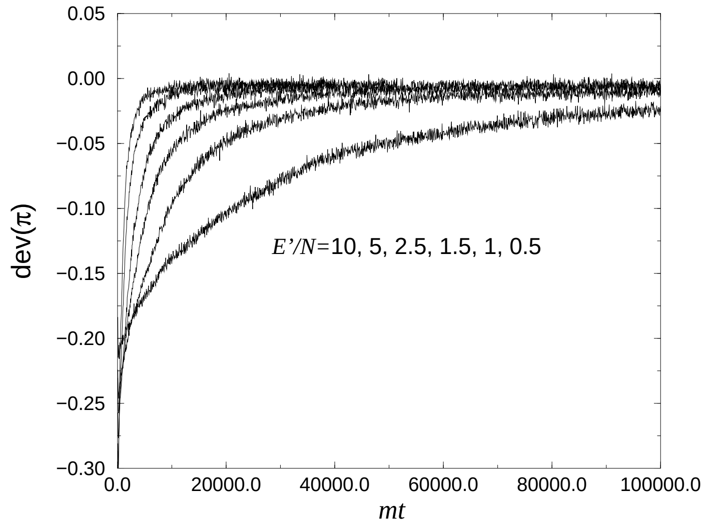

Figure 1: Time dependence of $\mathrm{dev}(\pi)_{\Delta t}$, averaged over $m\Delta t = 62.5$, for different values of the energy E'/N, from $E'/N = 10$ (top curve, fastest relaxation) to $E'/N = 0.5$ (bottom curve, slowest relaxation). Each curve represents the average over 20 independent initial conditions to reduce fluctuations. Parameters are $mL = 32, N = 256$.

is interesting for two reasons: first, although they never vanish, for a closed system one expects some suppression from the fact that the total energy is conserved. Second, one can calculate in the canonical case the size of the fluctuations exactly: $\mathrm{fluc}(K_s)_T = 2/N_s$. This provides the possibility for a quantitative comparison. The last observable we discuss is the normalized third moment of the kinetic energy in a subvolume (the second moment is related to $\mathrm{fluc}(K_s)$), and is denoted as

$$\mathrm{mom}(K_s^3) = \frac{\langle K_s^3 \rangle}{\langle K_s \rangle^3}. \tag{13}$$

In thermal equilibrium $\mathrm{mom}(K_s^3)_T = 1 + 6/N_s + 8/N_s^2$. This observable differs from the previous ones in that it is neither directly related to fluctuations nor purely local, since it involves the expectation value of $\langle \pi^2(x,t)\pi^2(y,t)\pi^2(z,t) \rangle$ with x, y, z all in the same subvolume. These three observables are related in a nonlinear manner to ensemble averages, and hence examples of "secondary" quantities. Note also that in the canonical ensemble they are independent of the temperature.

3 Single microstates

We start with ensembles consisting of one microstate only. For each E'/N we generate a number of initial conditions with the same energy, and integrate the

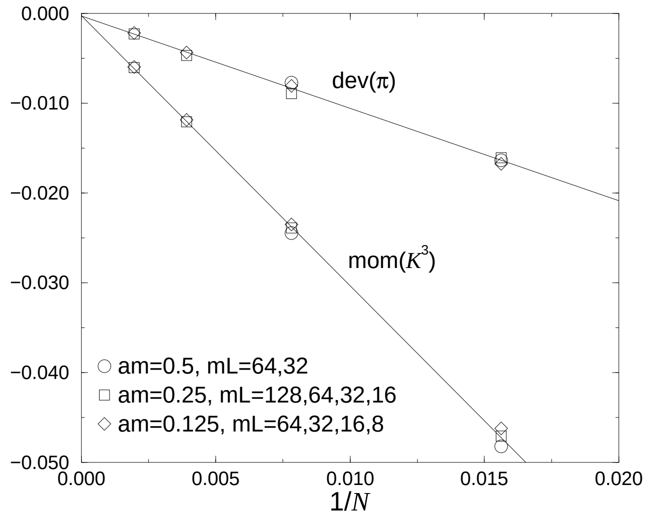

Figure 2: Dependence of $\mathrm{dev}(\pi)_{\Delta t}$ and the relative deviation of $\mathrm{mom}(K^3)_{\Delta t}$ from the thermal value on the number of lattice points N, in the quasi-stationary regime with $m\Delta t = 10000$, for various values of mL and ma. No significant dependence on the subvolume size or E'/N has been found. The lines are straight-line fits and statistical errors are smaller than the symbol sizes.

equation of motion. We take time averages over an interval Δt for each microstate separately. For convenience we sometimes average at the end over independent runs in order to reduce the fluctuations in time.

To get some feeling for the time scales involved, we show in Fig. 1 how $\mathrm{dev}(\pi)_{\Delta t}$ relaxes towards zero as a function of time, for various values of the energy. In this case the time averages are taken over an interval $m\Delta t = 62.5$, and since the size of the fluctuations in time in each microstate remains rather large, we show in Fig. 1 curves averaged over 20 independent initial conditions per energy value. As stated before, there is a correspondence between high energy and large coupling, and we see that the time scale involved increases for decreasing E'/N, as expected.

It is clear from Fig. 1 that π tends to become gaussian: $\mathrm{dev}(\pi)_{\Delta t} \to 0$. To make this precise, we discard the initial part where $\mathrm{dev}(\pi)_{\Delta t}$ is not quasi-stationary and calculate the time average in a long, interval $m\Delta t = 10000$, for several values of mL and ma, subvolume sizes $mL_s = 4, 8, 16$, and energies $E'/N = 2, \ldots, 10$. For each E'/N we have generated 10 initial conditions. We have observed no significant dependence of the long-time values on either the initial condition for a fixed energy, the energy E'/N in the interval indicated, or the subvolume size. The asymptotic average value of $\mathrm{dev}(\pi)_{\Delta t}$ depends only on the total number of degrees of freedom N, as shown in Fig. 2. Note that changing mL with fixed am or vice versa has the same effect. For finite N, we see that π deviates from being gaussian, on the order of a percent for $N = 100$. However, in

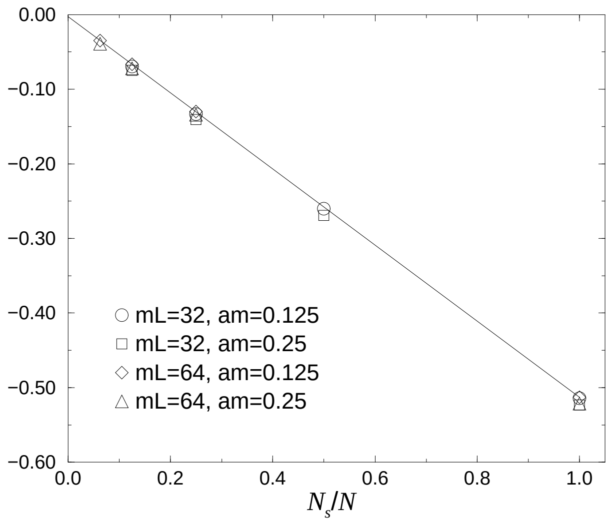

Figure 3: Relative deviation of $\mathrm{fluc}(K_s)_{\Delta t}$ from the thermal value, as a function of $L_s/L = N_s/N$, with $mL_s = 4, 8, 16$, for various values of mL and ma. The line is a straight-line fit through the $mL = 64, am = 0.125$ points.

the thermodynamic limit, which is $N \to \infty$ in this classical lattice model, π becomes a gaussian field. A straight-line fit shows that the thermodynamic limit is approached as $\mathrm{dev}(\pi)_{\Delta t} = -1.03(2)/N - 0.0003(2)$, where the numbers between brackets indicate the error in the last digit from the fit. Also shown in Fig. 2 is the relative deviation of $\mathrm{mom}(K^3)_{\Delta t}$ from the thermal value. Again we found no significant dependence on the subvolume size, the energy, or the particular initial condition. Also in this case we see a deviation from the thermal value for finite N, which vanishes in the thermodynamic limit as $-3.01(3)/N - 0.0003(3)$.

The relative deviation of $\mathrm{fluc}(K)_{\Delta t}$ from the thermal value is shown in Fig. 3, again in the quasi-stationary regime with $m\Delta t = 10000$, using several energies as before. We present the result as a function of $L_s/L = N_s/N$. For $N_s/N = 1$, we see that the fluctuations are suppressed by approximately 50%, compared to the thermal value. A straight-line fit shows that the data are consistent with

$$\mathrm{fluc}(K_s)_{\Delta t} = \frac{2}{N_s}\left(1 - \frac{1.4(2)}{N} - 0.514(1)\frac{N_s}{N}\right). \tag{14}$$

In other words, in the proper thermodynamic limit, $N \to \infty$ and $N_s/N \to 0$, the fluctuations are given by the canonical ones. On the other hand, in the limit $N \to \infty$ with *fixed* N_s/N, $\mathrm{fluc}(K_s)_{\Delta t}$ deviates from the canonical value, confirming the expectation that the heat bath must be infinitely larger than the subsystem under consideration.

The results obtained so far indicate that single microstates evolving from an initial condition taken from the class (5) thermalize in the thermodynamic limit, in a time-averaged sense.

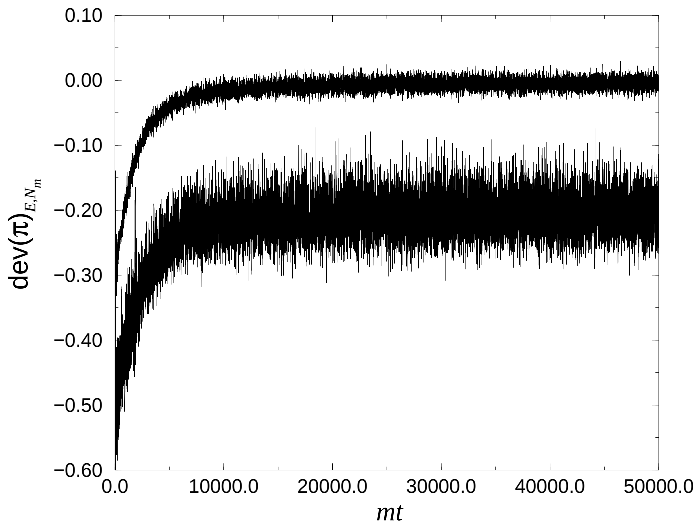

Figure 4: Time dependence of $\text{dev}(\pi)_{E,N_m}$ in nonequilibrium ensembles with $N_m = 10$ members (lower curve, shifted down by 0.2 for clarity) and $N_m = 150$ members (upper curve). In a larger ensemble the size of fluctuations is reduced. Parameters are $mL = 32, N = 256, E'/N = 4$.

4 Fixed-energy ensembles

To extend the analysis, we continue with fixed-energy ensembles, built as superpositions of $N_m > 1$ microstates (5) with the same energy E. We present the effect of ensemble averaging for $\text{dev}(\pi)_{E,N_m}$ in Fig. 4 for ensembles consisting of $N_m = 10$ and $N_m = 150$ members, respectively. We emphasize that there is no time averaging performed here, unlike the microstate case. It is seen that the larger the ensemble, the smaller the size of the fluctuations. To make this quantitative, we identify the size of the fluctuations with the standard deviation σ_{E,N_m} around the mean value in the quasi-stationary regime. Explicitly, for a generic primary observable

$$\sigma^2_{E,N_m} \equiv \left\langle \langle O \rangle^2_{E,N_m} \right\rangle_{\Delta t} - \left\langle \langle O \rangle_{E,N_m} \right\rangle^2_{\Delta t}. \tag{15}$$

In Fig. 5 we show the asymptotic values of σ_{E,N_m} for the observables T_π and $\text{dev}(\pi)$, as functions of $1/\sqrt{N_m}$. For the quasi-stationary regime the interval $30000 < mt < 50000$ was used. We see that in an ensemble with $N_m \to \infty$ members the standard deviations vanish, which implies that the expectation values become time-independent, and the ensemble becomes stationary.

These results are consistent with the results obtained in ensembles consisting of one microstate only. Using definition (2) for a primary observable O, we find

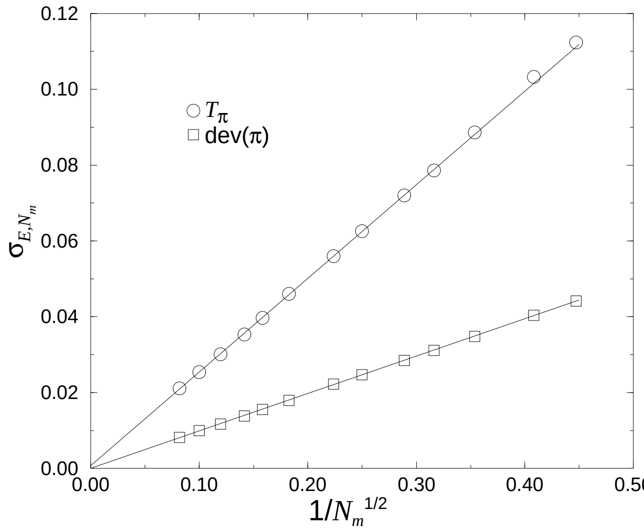

Figure 5: Size of the fluctuations σ_{E,N_m} for T_π and $\mathrm{dev}(\pi)$ versus $1/\sqrt{N_m}$, where N_m denotes the number of members in a fixed-energy ensemble, ranging from 5 to 150. The lines are straight-line fits through the eight lowest points. Same parameters as in Fig. 4.

that the variance (15) is given by

$$\begin{aligned} \sigma^2_{E,N_m} &= \frac{1}{N_m^2}\sum_{i,j}\left[\langle O_i O_j\rangle_{\Delta t}(t) - \langle O_i\rangle_{\Delta t}(t)\langle O_j\rangle_{\Delta t}(t)\right] \\ &= \frac{1}{N_m^2}\sum_{i}\left[\langle O_i^2\rangle_{\Delta t}(t) - \langle O_i\rangle^2_{\Delta t}(t)\right] \\ &= \frac{1}{N_m^2}\sum_{i}\sigma^2_{\Delta t,i}, \end{aligned} \tag{16}$$

where $\sigma_{\Delta t,i}$ denotes the standard deviation around the mean value in the quasi-stationary regime in the ith microstate. The second line follows if the individual microstates are statistically independent, i.e. $\langle O_i O_j\rangle_{\Delta t}(t) = \langle O_i\rangle_{\Delta t}(t)\langle O_j\rangle_{\Delta t}(t)$ for $i \neq j$. If we now use that the standard deviation $\sigma_{\Delta t,i}$ in a particular realization is independent of the specific details of the initial condition, such that $\sigma_{\Delta t,i} \equiv \sigma_{\Delta t}$ for all i, we conclude that $\sigma_{E,N_m} = \sigma_{\Delta t}/\sqrt{N_m}$, in agreement with the numerical results. Note that this implies that the initial probability distribution given by (5) with $n_\mathrm{e} = 4$ is already "rich" enough to define a fixed-energy ensemble with stationary asymptotic behaviour.

5 Generic ensembles

Perhaps surprisingly, we can use the results obtained above to show that generic ensembles approach noncanonical stationary distributions. Let us consider an

initial ensemble whose energy is not precisely fixed, but has some finite spread: $\Delta E^2 \equiv \langle (E - \langle E \rangle)^2 \rangle \neq 0$. Note that the spread is conserved during time evolution. The issue of thermalization in this case is more complicated. To get some feeling for this, let us first consider the simple case of a superposition of fixed-energy ensembles weighted with a normalized gaussian function $f(E)$:

$$f(E) = \mathcal{N}_\kappa \exp\left[-\frac{1}{2}\kappa(E-\bar{E})^2/\bar{E}^2\right], \tag{17}$$

with $\mathcal{N}_\kappa = (\kappa/2\pi\bar{E}^2)^{1/2}$ and where κ is a large but finite constant in the thermodynamic limit. The energy spread for this ensemble is $\Delta E^2/\bar{E}^2 = 1/\kappa$. Under the assumption that the individual fixed-energy ensembles evolve to the corresponding microcanonical ones, the large-time asymptotic stationary values of all primary quantities can be obtained by folding the microcanonical ones with $f(E)$. It is then straightforward to compute also secondary quantities such as connected functions. Using definition (10) for the temperature T_π, we obtain[2]

$$\mathrm{dev}(\pi)_\kappa \approx 1/\kappa, \tag{18}$$

$$\langle \pi^2(x)\pi^2(y)\rangle_\kappa - \langle \pi^2(x)\rangle_\kappa \langle \pi^2(y)\rangle_\kappa \approx (T_\pi/a)^2/\kappa, \quad x \neq y. \tag{19}$$

We emphasize that secondary quantities defined for the whole ensemble are *not* weighted averages of the corresponding quantities in the individual microcanical ensembles. From Eq. (18) we see that this ensemble does not have thermal correlation functions, i.e. $\mathrm{dev}(\pi)_\kappa \neq 0$, not even in the thermodynamic limit. Furthermore, since the left-hand-side of Eq. (19) is nothing else than the connected four-point function and the right-hand-side does not vanish for $|x-y| \to \infty$, we find that the ensemble (17) does not obey the clustering property [11]. A violation of clustering has a rather large impact on other observables, for instance for $N \gg N_s$ we find that

$$\mathrm{fluc}(K_s)_\kappa = \frac{2}{N_s}\left(1 + \frac{N_s+2}{2\kappa}\right). \tag{20}$$

Fluctuations in the kinetic energy in subvolumes will deviate substantially from the canonical value when $\kappa \sim N_s$. In the limit that $N_s \gg \kappa$, the size of the fluctuations approaches $1/\kappa$ and therefore does not vanish.

In order to make the discussion more general, let us now consider a system with n_c conserved *intensive* quantities $\mathbf{c} = \{c_\mu\}$, $\mu = 1, \ldots, n_c$. Supported by our numerical results, we assume that all microstates with given $\mathbf{c}$ evolve, in an asymptotic, time-averaged sense, to the same final state, i.e. that all details of the initial state other than the conserved quantities are lost. In other words, for a local observable O in microstate i:

$$\lim_{t\to\infty, \Delta t\to\infty, \Delta t/t\to 0} \frac{1}{\Delta t}\int_{t-\Delta t}^{t} O_i(t) = \langle O \rangle^*_{N,\mathbf{c}}. \tag{21}$$

[2]Neglecting the nonlinear T-dependence of E.

Here $\langle O\rangle^*_{N,\mathbf{c}}$ is the expectation value of O in the microcanonical ensemble with fixed $\mathbf{c}$ and N degrees of freedom.[3] We further assume that an ensemble consisting of a superposition of sufficiently many states, all with the same values of $\mathbf{c}$, evolves to the corresponding microcanonical ensemble:

$$\lim_{t\to\infty}\langle O(t)\rangle_{\mathbf{c}} = \langle O\rangle^*_{N,\mathbf{c}}. \tag{22}$$

Notice that in this case no time averaging is required.

We then consider ensembles that are superpositions of states with different values of $\mathbf{c}$, weighted with a normalized weight function $f_N(\mathbf{c})$. As an example, one may consider again a gaussian distribution:

$$f_N(\mathbf{c}) = \prod_\mu \frac{1}{\sqrt{2\pi\Delta c_\mu^2}} \exp\left[-\frac{1}{2}(c_\mu - \overline{c}_\mu)^2/\Delta c_\mu^2\right],$$

with $\Delta c_\mu \sim 1/N^\alpha$. In this case $\Delta\mathbf{c}^2 \equiv \overline{\mathbf{c}^2} - \overline{\mathbf{c}}^2 \neq 0$, where $\overline{\mathbf{c}} = \int d\mathbf{c}\, f_N(\mathbf{c})\mathbf{c}$. Provided that the ensemble is sufficiently "rich", i.e. all subensembles with given values of $\mathbf{c}$ satisfy Eq. (22), the asymptotic expectation values depend only on the weight function $f_N(\mathbf{c})$:

$$\langle O\rangle^*_{f_N} = \int d\mathbf{c}\; f_N(\mathbf{c})\langle O\rangle^*_{N,\mathbf{c}}. \tag{23}$$

For $\Delta c_\mu \sim 1/N^\alpha$ we extract the leading N-dependence by writing the weight function f_N as

$$f_N(\mathbf{c}) = N^{\alpha n_c}\varphi(\mathbf{s}), \quad \mathbf{s} = N^\alpha(\mathbf{c}-\overline{\mathbf{c}}), \tag{24}$$

where we assume that φ is in first approximation N-independent. The case $\alpha = 0$ corresponds to fixed $\Delta c_\mu/c_\mu$, independent of N. For a canonical ensemble one has $f_N^{\mathrm{can}}(E/N) = Z_T^{-1}\Omega(E)e^{-E/T}$, where $\Omega(E)$ is the number of states with energy density $\epsilon = E/N$ and Z_T is the canonical partition function. In this case, the spread in the energy density is given by $\Delta\epsilon \sim N^{-1/2}$ and therefore $\alpha = 1/2$. In general, we shall assume $\alpha \geq 0$.

We expand $\langle O\rangle^*_{N,\mathbf{c}}$ in a Taylor series around $\overline{\mathbf{c}}$ such that Eq. (23) yields

$$\begin{aligned}\langle O\rangle^*_{f_N} &= \sum_{m=0}^{\infty}\frac{1}{m!N^{\alpha m}}\frac{\partial^m\langle O\rangle^*_{N,\overline{\mathbf{c}}}}{\partial c_{\mu_1}\dots\partial c_{\mu_m}}\int d\mathbf{s}\,\varphi(\mathbf{s})s_{\mu_1}\dots s_{\mu_m}\\ &= \langle O\rangle^*_{N,\overline{\mathbf{c}}} + \frac{\overline{s_\mu s_\nu}}{2N^{2\alpha}}\frac{\partial^2\langle O\rangle^*_{N,\overline{\mathbf{c}}}}{\partial c_\mu\partial c_\nu} + \mathcal{O}(N^{-3\alpha}),\end{aligned} \tag{25}$$

with $\overline{s_\mu s_\nu} = \int d\mathbf{s}\,\varphi(\mathbf{s})s_\mu s_\nu$. Notice that the $m=1$ term in the series drops out due to the definition of $\overline{\mathbf{c}}$. In the case that f_N is the weight function for the canonical ensemble, Eq. (25) shows that the expectation values in a fixed-energy ensemble

[3]Asymptotic values will generically be denoted with a star.

will differ from the canonical ones as $\sim 1/N$. This is exactly the behaviour we found numerically (see above). Generic ensembles with $\alpha > 0$ can be compared with the canonical one by applying (25) twice, i.e. by subtracting from (25) the same equation with $f_N = f_N^{\rm can}$. It is then found that primary observables, i.e. expectation values that are directly given as ensemble averages, approach the canonical values in the thermodynamic limit, and the way this limit is approached is directly proportional to the spread in the conserved quantities $\overline{s_\mu s_\nu}$. For a finite $\Delta c_\mu / c_\mu$ in the thermodynamic limit, the asymptotic expectation values will differ by a nonzero amount from both the microcanonical and the canonical ensembles, even in the thermodynamic limit. However, this difference is suppressed by Δc^2.

For secondary quantities, i.e. observables that are nonlinear functions of ensemble averages, the situation is more involved. For definiteness, let us go back to the scalar theory (3), which has only one conserved quantity: $c_1 = \epsilon$.[4] We restrict ourselves to translation-invariant ensembles. Notice also that the connected two-point functions for ϕ and π behave asymptotically as primary quantities, since $\langle \phi \rangle_N^* = \langle \pi \rangle_N^* = 0$. An example of a secondary quantity is the equal-time connected 4-point correlation function

$$\begin{aligned}\langle \psi(x)\psi(y)\psi(z)\psi(w)\rangle_{f_N,C} \;\equiv\;& \langle \psi(x)\psi(y)\psi(z)\psi(w)\rangle_{f_N} \\ & - \left(\langle \psi(x)\psi(y)\rangle_{f_N}\langle \psi(z)\psi(w)\rangle_{f_N} + \textit{two perm.}\right),\end{aligned} \tag{26}$$

with $\psi = \{\pi, \phi\}$. Here we have extended the standard definition of connected correlation functions to arbitrary ensembles. In particular, $\langle \pi^4(x)\rangle^*_{f_N,C}$ is related to dev(π) in Eq. (11). Using Eq. (25), we find

$$\langle \pi^4(x)\rangle^*_{f_N,C} \approx \langle \pi^4(x)\rangle^*_{N,\bar\epsilon,C} + \frac{\overline{s^2}}{2N^{2\alpha}}\left[\frac{d^2}{d\epsilon^2}\langle \pi^4(x)\rangle^*_{N,\bar\epsilon,C} + 6\left(\frac{d}{d\epsilon}\langle \pi^2(x)\rangle^*_{N,\bar\epsilon}\right)^2\right], \tag{27}$$

with $\overline{s^2}/N^{2\alpha} = \Delta\epsilon^2$. In the case that $f_N = f_N^{\rm can}$ (with $\alpha = 1/2$), the connected 4-point function on the left-hand-side vanishes, and the fluctuations in the energy density are given by $\overline{s^2} = T^2 \partial\bar\epsilon/\partial T$. If we use the definition of temperature in the fixed-energy ensemble $T_\pi/a = \langle \pi^2(x)\rangle^*_{N,\bar\epsilon}$ and work consistently to order $1/N$, so that T_π can be identified with the temperature T in the canonical ensemble, Eq. (27) yields

$$\langle \pi^4(x)\rangle^*_{N,\bar\epsilon,C} = -3\frac{\overline{s^2}}{N}\left(\frac{d}{d\epsilon}\langle \pi^2(x)\rangle^*_{N,\bar\epsilon}\right)^2 = -\frac{3}{N}\left(\frac{T}{a}\right)^2\frac{\partial T}{\partial\bar\epsilon}, \tag{28}$$

and

$$\mathrm{dev}(\pi)_E = \frac{\langle \pi^4(x)\rangle^*_{N,\bar\epsilon,C}}{3\langle \pi^2(x)\rangle^{*2}_{N,\bar\epsilon}} = -\frac{1}{N}\frac{\partial T}{\partial\bar\epsilon}. \tag{29}$$

[4]The other obvious candidate, the total momentum $P = \sum_x \pi(x)\partial_x\phi(x)$, is not conserved on the lattice. We have checked that expectation values of P and P^2 approximately thermalize, regardless of their initial values.

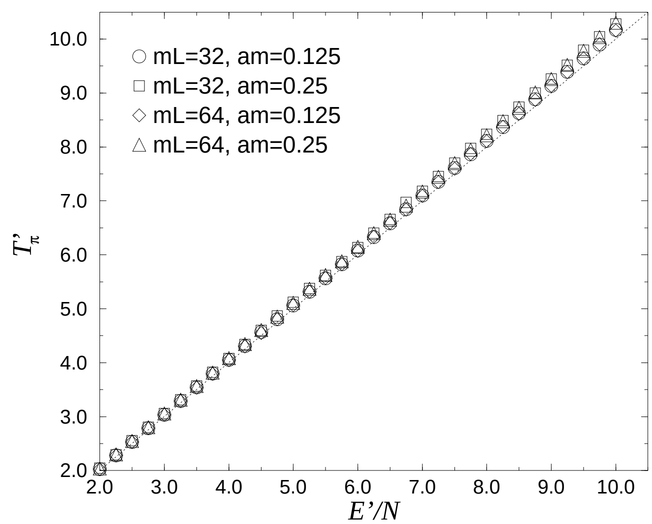

Figure 6: Dependence of the effective temperature T'_π on the energy density E'/N, for several values of ma and mL. The dashed line is the free ($\lambda = 0$) relation.

We have measured dev(π) and the energy dependence of the effective temperature in fixed-energy ensembles independently (Figs. 2 and 6, respectively), and have found Eq. (29) to be satisfied within numerical accuracy.

As we saw in the example (17), the connected function (26) does not, in general, obey the clustering property. Using Eq. (25), we can write

$$\langle\psi^2(x)\psi^2(y)\rangle^*_{f_N,C} \approx \langle\psi^2(x)\psi^2(y)\rangle^*_{N,\bar{\epsilon},C} + \frac{\overline{s^2}}{2N^{2\alpha}}\left[\frac{d^2}{d\epsilon^2}\langle\psi^2(x)\psi^2(y)\rangle^*_{N,\bar{\epsilon},C} + 2\left(\frac{d}{d\epsilon}\langle\psi^2(x)\rangle^*_{N,\bar{\epsilon}}\right)^2 + 4\left(\frac{d}{d\epsilon}\langle\psi(x)\psi(y)\rangle^*_{N,\bar{\epsilon}}\right)^2\right]. \quad (30)$$

The limit of large spatial separation for the fixed-energy ensembles can be extracted by comparison with the canonical ensemble, where clustering holds and the left-hand-side vanishes for $|x-y| \to \infty$. Using $f_N = f_N^{\rm can}$, one finds

$$\lim_{|x-y|\to\infty}\langle\psi^2(x)\psi^2(y)\rangle^*_{N,\bar{\epsilon},C} = -\frac{T^2}{N}\frac{\partial\bar{\epsilon}}{\partial T}\left(\frac{d}{d\epsilon}\langle\psi^2(x)\rangle^*_{N,\bar{\epsilon}}\right)^2 + \mathcal{O}(N^{-3/2}). \quad (31)$$

In the microcanonical ensemble the connected 4-point function vanishes, in the limit of large separations, only up to terms of order $1/N$. Using this result in Eq. (30) for an generic ensemble with a nonzero (noncanonical) spread in the energy density, we find that also in these ensembles the clustering property will be violated. For $\alpha = 0$ the right-hand-side of Eq. (30) is dominated by the first term on the second line and we recover the result (19).

It is instructive to translate these findings to momentum space. We introduce the notation

$$\langle\psi(q_1)\ldots\psi(q_n)\rangle \equiv Na\delta_{q_1+\ldots+q_N,0}\langle\langle\psi_1\ldots\psi_n\rangle\rangle \tag{32}$$

where we factored out a Kronecker delta function times the volume to take translational invariance into account. For a clustering system, all reduced connected functions $\langle\langle\ldots\rangle\rangle$ should be finite in the limit $N\to\infty$, a fixed. For the connected 4-point function of a generic ensemble we have

$$\begin{aligned}\langle\langle\psi_1\psi_2\psi_3\psi_4\rangle\rangle^*_{f_N,C} &= \langle\langle\psi_1\psi_2\psi_3\psi_4\rangle\rangle^*_{f_N} - Na\left(\langle\langle\psi_1\psi_2\rangle\rangle^*_{f_N}\langle\langle\psi_3\psi_4\rangle\rangle^*_{f_N}\delta_{q_1,-q_2} + perm.\right)\\ &= \langle\langle\psi_1\psi_2\psi_3\psi_4\rangle\rangle^*_{N,\bar\epsilon,C} + \frac{\overline{s^2}}{2N^{2\alpha}}\frac{d^2}{d\epsilon^2}\langle\langle\psi_1\psi_2\psi_3\psi_4\rangle\rangle^*_{N,\bar\epsilon,C}\\ &\quad+\frac{\overline{s^2}a}{N^{2\alpha-1}}\left[\frac{d}{d\epsilon}\langle\langle\psi_1\psi_2\rangle\rangle^*_{N,\bar\epsilon}\frac{d}{d\epsilon}\langle\langle\psi_3\psi_4\rangle\rangle^*_{N,\bar\epsilon}\delta_{q_1,-q_2} + perm.\right].\end{aligned} \tag{33}$$

When momenta come in pairs, the reduced connected 4-point functions for the microcanonical and canonical ensembles differ even in the thermodynamic limit, and, remarkably, for ensembles with $\alpha < 1/2$ these functions actually diverge. A similar calculation for the connected 6-point function gives, to leading order,

$$\begin{aligned}\langle\langle\psi_1\ldots\psi_6\rangle\rangle^*_{f_N,C} &= \langle\langle\psi_1\ldots\psi_6\rangle\rangle^*_{N,\bar\epsilon,C}\\ &+\frac{\overline{s^2}a^2}{N^{2\alpha-2}}\left[\langle\langle\psi_1\psi_2\rangle\rangle^*_{N,\bar\epsilon}\frac{d}{d\epsilon}\langle\langle\psi_3\psi_4\rangle\rangle^*_{N,\bar\epsilon}\frac{d}{d\epsilon}\langle\langle\psi_5\psi_6\rangle\rangle^*_{N,\bar\epsilon}\delta_{q_1,-q_2}\delta_{q_3,-q_4} + perm.\right].\end{aligned} \tag{34}$$

A comparison with the canonical ensemble shows that the reduced connected 6-point function in the microcanonical ensemble diverges in the thermodynamic limit $\sim N$. For higher order connected functions to be finite for all momentum combinations, f_N has to agree with f_N^{can} to higher and higher order in $1/N$. Approximation methods based on expansions in connected or 1-particle irreducible correlation functions may break down since higher-point functions could strongly affect the expansion. Without taking care of the failure of clustering properties they may not be suitable to describe thermalization phenomena. This might explain some qualitatively different results obtained in [9, 10], where the same scalar theory was studied using truncations of an exact flow equation for the time evolution of equal-time correlation functions [8]. It also puts doubts on the validity of approximations which lead to thermalization for arbitrary initial ensembles.

6 Conclusion

Let us summarize our conclusions for the time evolution of classical ensembles with nonequilibrium initial conditions, based on numerical results for the ϕ^4 theory in $1+1$ dimensions on the lattice. The investigated statistical ensembles approach in the large-time limit stationary ensembles that depend only on the

probability distribution for the energy density (and the other intensive conserved quantities). For ensembles that consist of a small number of microstates, the asymptotic ensemble is approached only in a time-averaged sense. For a very large number of degrees of freedom (thermodynamic limit) we find that ensembles with a nonzero energy density spread do not approach the canonical ensemble: their large-time primary observables differ from the thermal values by a finite amount proportional to the spread. Ensembles with vanishing spread, on the other hand, do thermalize, up to terms suppressed by the number of degrees of freedom. These corrections can be computed, and our numerical results were found to be in excellent agreement with the analytical results.

We also notice that generic statistical ensembles do not cluster for large time. Secondary quantities (like connected or 1PI functions) receive corrections that in coordinate space do not vanish in the limit of large spatial separation; as a result, corrections to quantities defined over large subvolumes can be very large. In momentum space, violation of clustering implies that for specific momentum values secondary quantities diverge in the thermodynamic limit. Clustering requires a vanishing initial spread in all conserved quantities with extreme precision. We argue therefore that care should be exercised when applying approximate methods based on expansions in connected or 1-particle irreducible correlation functions to the study of thermalization: such methods might in fact break down in the large-time regime.

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